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1. REPORT DATE (DD-MM-YYYY) 17-04-2015		2. REPORT TYPE Final Report		3. DATES COVERED (From - To) 5-Apr-2013 - 4-Oct-2013	
4. TITLE AND SUBTITLE Final Report: Symposium on Energy Storage Materials Energy and Fuel Division, 246th ACS National Meeting			5a. CONTRACT NUMBER W911NF-13-1-0077		
			5b. GRANT NUMBER		
			5c. PROGRAM ELEMENT NUMBER 611102		
6. AUTHORS Shirley Meng			5d. PROJECT NUMBER		
			5e. TASK NUMBER		
			5f. WORK UNIT NUMBER		
7. PERFORMING ORGANIZATION NAMES AND ADDRESSES University of California - San Diego Office of Contract & Grant Adm 9500 Gilman Drive, 0934 La Jolla, CA 92093 -0934			8. PERFORMING ORGANIZATION REPORT NUMBER		
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES) U.S. Army Research Office P.O. Box 12211 Research Triangle Park, NC 27709-2211			10. SPONSOR/MONITOR'S ACRONYM(S) ARO		
			11. SPONSOR/MONITOR'S REPORT NUMBER(S) 64015-CH-CF.1		
12. DISTRIBUTION AVAILABILITY STATEMENT Approved for Public Release; Distribution Unlimited					
13. SUPPLEMENTARY NOTES The views, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy or decision, unless so designated by other documentation.					
14. ABSTRACT The symposium took place on September 10th 2013 and lasted for two and half days. We had excellent attendance throughout the entire meeting. This symposium as part of Energy and Fuel Division (ENFL) aimed to bring together chemical scientists of various areas to present their research on energy storage materials. The final invited speakers included Dr. Daniel Steingart (Princeton University), Dr. Gao Liu (Lawrence Berkeley Lab), Dr. Yat Li (University of California Santa Cruz), Dr. Arumugam Manthiram (University of Texas, Austin), Dr. Peter Faguy (DOE/ATO) and Dr. Bruce Dunn (University of California Los Angeles). In the three day symposium, 25 oral					
15. SUBJECT TERMS ARO, symposium, batteries, energy, ACS					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT UU	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON Shirley Meng
a. REPORT UU	b. ABSTRACT UU	c. THIS PAGE UU			19b. TELEPHONE NUMBER 858-822-4247

Report Title

Final Report: Symposium on Energy Storage Materials Energy and Fuel Division, 246th ACS National Meeting

ABSTRACT

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Final Report on the ARO funding support for symposium “Advances in Batteries, Capacitors, and other Energy Storage Devices” in 246th, American Chemical Society Biannual Meeting in Indianapolis. September 8-12, 2013.

Prepared by Shirley Meng, Department of NanoEngineering, UC San Diego

The symposium took place on September 10th 2013 and lasted for two and half days. We had excellent attendance throughout the entire meeting. This symposium as part of Energy and Fuel Division (ENFL) aimed to bring together chemical scientists of various areas to present their research on energy storage materials. The final invited speakers included Dr. Daniel Steingart (Princeton University), Dr. Gao Liu (Lawrence Berkeley Lab), Dr. Yat Li (University of California Santa Cruz), Dr. Arumugam Manthiram (University of Texas, Austin), Dr. Peter Faguy (DOE/VTO) and Dr. Bruce Dunn (University of California Los Angeles). In the three day symposium, 25 oral presentations were given, covering topics from cathode and anode materials, electrolytes and interfaces, computation, diagnostics and evaluations, as well as advanced characterization techniques.

The detailed online published abstracts of all oral presentations are attached in the following pages.

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Division of Energy and Fuels American Chemical Society Symposium

Symposium on

Advances in Batteries, Capacitors, and Other Energy Storage Devices

246th ACS National Meeting & Exposition, September 8-12, 2013

Indianapolis, Indiana

This Symposium features recent advances and/or new developments in the area of Energy Storage Technology. Topics include, but are not limited to:

- **Novel Electrode Materials for Batteries and Capacitors**
- **Computational Materials Design and Engineering**
- **Flexible Energy Storage Devices**
- **Electrode/Electrolyte Interface Phenomena**
- **Advanced Characterization Techniques**
- **New Electrolyte Materials**
- **Large-scale Fabrication and Assembly Technology**
- **Other Energy Storage Devices and Systems**

Confirmed Invited Speakers

- **K. Amine**, Argonne National Laboratory
- **B. Dunn**, University of California, Los Angeles
- **S. Harris**, Lawrence Berkeley National Laboratory
- **J. Liu**, Pacific Northwest National Laboratory
- **A. Manthiram**, University of Texas at Austin
- **J. Zhang**, Argonne National Laboratory
- **Y. Li**, University of California, Santa Cruz
- **D. Steingart**, Princeton

Organizers

- **Prof. Shirley Meng**, NanoEngineering, University of California, San Diego, CA 92121, Phone: 858-822-4247, Email: shirleymeng@ucsd.edu
- **Dr. Kang Xu**, Electrochemistry Branch, U. S. Army Research Laboratory, Adelphi, MD 20783, Phone: 301-394-0321, email: Conrad.k.xu.civ@mail.mil
- **Prof. Mark A. Allen**, Department of Chemistry and Biochemistry, University of Maryland, Baltimore County, Baltimore, MD 21250, Phone: 410-455-2539, Email: allenm@umbc.edu
- **Prof. Guihua Yu**, Department of Mechanical Engineering, The University of Texas at Austin, Austin, TX 78712, Phone: 512-232-5276, Email: ghyu@austin.utexas.edu

Abstract and pre-print submission due date: April 1st, 2013

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Program Co-Chair

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246th ACS National Meeting and Exposition
September 8-12, 2013, Indianapolis, Indiana

Divisions

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ENFL

Ranjit Koodali, Yun Hu

Tuesday, September 10, 2013

Oral Session

Advances in Batteries, Capacitors, and other Energy Storage Devices - PM Session

Li-Ion batteries: Cathodes and Spectroscopic Studies

Location: Indiana Convention Center

Room: 123

Organizers: Kang Xu, Shirley Meng, Guihua Yu, Mark Allen

Presiders: Guihua Yu, Shirley Meng

Duration: 1:00 pm - 4:55 pm

Pres Time	Pub #	Presentation Title
1:00 pm		Introductory Remarks
1:05 pm	294	Applied research at the US DOE supporting the development of next-generation batteries for plug-in electric vehicles (PEVs) Peter Faquy
1:45 pm	295	Phosphate and diphosphate bimetallic cathode materials Esther Sans Takeuchi , Amy C Marschilok, Kenneth J Takeuchi.
2:15 pm	296	Toward fully plastic batteries: Electroactive polymer-carbon composite electrode as cathode material for rechargeable batteries Burak Esat , Muhammed Aydin.
2:35 pm	297	Thermal-induced decomposition roadmap of charged cathode material $\text{Li}_{1.2-x}\text{Ni}_{0.15}\text{Co}_{0.1}\text{Mn}_{0.55}\text{O}_2$ studied by synchrotron X-ray techniques Chi-Kai Lin , Yang Ren, Ira Bloom, Zonghai Chen.
2:55 pm		Intermission
3:05 pm	298	High-voltage cathodes for lithium-ion batteries Arumugam Manthiram , Katharine Chemelewski.
3:45 pm	299	Probing electrochemical cycling stability of oxide cathode materials for Li-ion batteries by advanced electron microscopy Miaofang Chi , Danna Qian, Christopher Fell, Shirley Meng.
4:15 pm	300	Study of phase changes about LiFePO_4 cathode in an 18650 commercial cell: An in situ time-resolved high energy synchrotron XRD study Qi Liu , Yang Ren, Jian Xie.
4:35 pm	301	WITHDRAWN

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Ranjit Koodali, Yun Hu

Wednesday, September 11, 2013

Oral Session

Advances in Batteries, Capacitors, and other Energy Storage Devices - AM Session

Li-Ion Batteries: Anodes and Electrolytes

Location: Indiana Convention Center

Room: 123

Organizers: Kang Xu, Shirley Meng, Guihua Yu, Mark Allen

Presiders: Mark Allen, Selena Russell, Shirley Meng

Duration: 8:00 am - 12:10 pm

Pres Time	Pub #	Presentation Title
8:00 am	394	Development of conductive binders for Si and tin anodes Gao Liu
8:40 am	395	Understanding Li-ion batteries failure from first-principles calculations: The effect of lithiation on the Si/Cu interface in Si anodes Maria E Stournara , Priya Johari , Yue Qi , Vivek B Shenoy .
9:00 am	396	Electrochemical characterization Li-ion battery Sn anodes Anne Co , Danny Liu , Jennifer Black , Amy Casaday .
9:20 am	397	Applications of carbide-derived carbon as electrodes for rechargeable lithium-ion batteries Sun-Hwa Yeon , Kyu-Nam Jung , Sukeun Yoon , Kyoung-Hee Shin , Jae-Deok Jeon .
9:40 am	398	Capturing the interface in Li-ion cells with heavy alkali dopants: Raman and X-ray techniques Christopher J Patridge , Corey T Love , David E Ramaker .
10:00 am		Intermission
10:10 am	399	Mn dissolution induced surface related battery degradation and method to mitigate by simple surface treatment Steve Harris , Chen Li .
10:50 am	400	High voltage electrolyte based on fluorinated compounds for 5V Li-ion chemistry Zhengcheng Zhang , Libo Hu , Huiming Wu , Khalil Amine .
11:20 am	401	Effect of electrolyte additives on solid electrolyte interphase properties in Li-ion batteries as analyzed by in-situ atomic force microscopy Arthur V. Cresce , David R. Baker , Selena M. Russell , Kang Xu .
11:50 am	402	Electrolytes for lithium batteries from oligo(ethylene glycol) functionalized cyclophosphazenes and phosphazene oligomers Kinkini Roy , Zhengcheng Zhang , Khalil Amine , E Bryan Coughlin .

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Ranjit Koodali, Yun Hu

Wednesday, September 11, 2013

Oral Session

Advances in Batteries, Capacitors, and other Energy Storage Devices - PM Session

Beyond Li-Ion Batteries

Location: Indiana Convention Center

Room: 123

Organizers: Kang Xu, Shirley Meng, Guihua Yu, Mark Allen

Presiders: Guihua Yu, Mark Allen, Shirley Meng

Duration: 1:00 pm - 5:15 pm

Pres Time	Pub #	Presentation Title
1:00 pm		Introductory Remarks
1:05 pm	447	Balanced approach for energy storage Jun Liu
1:45 pm	448	Anomalous manganese activation of a pyrophosphate cathode in sodium ion batteries: A combined experimental and theoretical study Chansun Park , Heejin Kim , Rara A. Shakoor , Eunjeong Yang , SooYeon Lim , Ramazan Kahraman , Yousung Jung , Jangwook Choi .
2:05 pm	449	Development of high energy density Li-organic redox flow battery Wei Wang , Wu Xu , Xiaoliang Wei , Lelia Cosimbescu , Daiwon Choi , Vincent Sprenkle .
2:25 pm	450	Electrodeposition of metal-air battery cathodes: Fabrication, characterization, and electrochemistry Amy C Marschilok , Shu Han Lee , Esther S Takeuchi , Kenneth J Takeuchi .
2:45 pm	451	Li intercalation capacity of Fe-phthalocyanine Ramos-Sanchez Guadalupe , Perla B Balbuena .
3:05 pm		Intermission

3:15 pm	452	Low cost, abundant, defective materials for large scale electrical energy storage Dan Steingart
3:45 pm	453	Fundamentals and structure designs for Na-ion battery anodes Liangbing Hu
4:15 pm	454	Enhanced lithium ion battery via biological engineering Scott J Riley
4:35 pm	455	WITHDRAWN
4:55 pm	456	WITHDRAWN

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Thursday, September 12, 2013

Oral Session

Advances in Batteries, Capacitors, and other Energy Storage Devices - AM Session

Capacitive Energy Storage Devices

Location: Indiana Convention Center

Room: 123

Organizers: Kang Xu, Shirley Meng, Guihua Yu, Mark Allen

Presiders: Mark Allen, Guihua Yu

Duration: 8:00 am - 11:25 am

Pres Time	Pub #	Presentation Title
8:00 am	505	Pseudocapacitive energy storage in 2D Nb₂O₅-graphene nanocomposites Guillaume Muller, Hyungseok Kim, Xavier Petrisans, Veronica Augustyn, Bruce Dunn .
8:40 am	506	High performance heterogeneous catalysis at ultrashort contact time for fuel cell cathode air using microfibrillar entrapped catalysts Qiang Gu , Bruce Tatarchuk.
9:00 am	507	Natural cellulose fiber as substrate for supercapacitor with extra ion diffusion pathway Zhe Gui , Hongli Zhu, Eleanor Gillette, Junkai Hu, Liangbing Hu, Sangbok Lee.
9:20 am		Intermission
9:30 am	508	Semiconductor nanowire-arrayed electrodes for supercapacitors Yat Li
10:00 am	509	Graphene-based composites as electrochemical supercapacitors Zhefei Li , Jian Xie.
10:20 am	510	WITHDRAWN
10:40 am	511	Mechanism of oxidized redox shuttle reduction at graphite or LTO anodes Mary Patterson
11:00 am	512	Synthesis of boron carbide, zirconium carbide, and niobium carbide nanofibers through electrospinning followed by carbothermal reduction Jennifer S Atchison , Volker Presser.
11:20 am		Concluding Remarks

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Ranjit Koodali, Yun Hu

Tuesday, September 10, 2013

294 - Applied research at the US DOE supporting the development of next-generation batteries for plug-in electric vehicles (PEVs)

Peter Faguy, peter.faguy@ee.doe.gov, Office of Energy Efficiency and Renewable Energy, Department of Energy, Washington, Washington DC 20585, United States

Translational science—R&D moving from the discovery/invention to societally beneficial devices and processes—has become a significantly larger, more manifest component of the Department of Energy's research portfolio. 'From the lab bench to the plant floor' has become a hallmark of the DOE's Office of Energy Efficiency and Renewable Energy, but no more so than for Sustainable Transportation. This talk will provide an overview of the technical aspects of FY2013+ programs in electrochemical energy storage supporting President Obama's EV-Everywhere Challenge. The initiative, which will bring together the Office of Energy Efficiency and Renewable Energy's Vehicle Technologies Office, the Office of Science's Basic Energy Sciences Program, and the Advanced Research Projects Agency — Energy (ARPA-E), exists to make electric vehicles affordable. Central to the initiative's larger mission is realizing the promise of next-generation Li-ion batteries for plug-in vehicles. The programmatic overview will be augmented with recent results addressing the critical performance issues with high voltage, high capacity Li-ion batteries.

Tuesday, September 10, 2013 01:05 PM[Advances in Batteries, Capacitors, and other Energy Storage Devices \(01:00 PM - 04:55 PM\)](#)**Location: Indiana Convention Center****Room: 123**

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Tuesday, September 10, 2013

295 - Phosphate and diphosphate bimetallic cathode materials

Esther Sans Takeuchi^{1,2,3}, esther.takeuchi@stonybrook.edu, Amy C Marschilok^{1,2}, Kenneth J Takeuchi¹. (1) Department of Chemistry, Stony Brook University, Stony Brook, NY 11794, United States, (2) Department of Materials Science and Engineering, Stony Brook University, Stony Brook, NY 11794, United States, (3) Global and Regional Solutions Directorate, Brookhaven National Laboratory, Upton, NY 11973, United States

Advances in energy storage materials have taken on expanded significance due to the needed ability to store electricity for many applications. Recently, the use of phosphate based materials has led to increased cathode stability, with a notable example being lithium iron phosphate, LiFePO_4 . While the voltage and energy density of phosphate based materials may be lower than oxide materials when used for lithium based systems, the chemical and electrochemical stability of the phosphate based materials are viewed as a significant asset. However, the inherently low electrical conductivity of phosphate materials must be addressed.

Bimetallic cathode materials have been employed in batteries partly because they can provide multiple electron reduction per formula unit. A notable example is the silver vanadium oxide ($\text{Ag}_2\text{V}_4\text{O}_{11}$) system used in biomedical batteries that power implantable cardiac defibrillators (ICDs). Lithium batteries using $\text{Ag}_2\text{V}_4\text{O}_{11}$ cathodes provide the opportunity for multiple electron reduction per $\text{Ag}_2\text{V}_4\text{O}_{11}$ formula unit. Additionally, an interesting aspect of silver vanadium oxide ($\text{Ag}_2\text{V}_4\text{O}_{11}$) is its ability to form *in-situ* silver metal nanoparticles upon reduction of Ag^+ to Ag^0 , contributing to the high electrical conductivity of partially discharged silver vanadium oxide.

We have embarked on the rational study of a new family of cathode materials for lithium batteries, namely silver vanadium phosphorous oxides ($\text{Ag}_w\text{V}_x\text{P}_y\text{O}_z$), with the broad goal of combining the thermal stability of lithium iron phosphate with the enhanced electrical conductivity of partially reduced silver vanadium oxide. Thus, enabling the use of phosphate based materials directly without the need for nanosizing or carbon coating.

Three members of the $\text{Ag}_w\text{V}_x\text{P}_y\text{O}_z$ family of compounds have been explored, $\text{Ag}_2\text{VO}_2\text{PO}_4$, $\text{Ag}_{0.48}\text{VOPO}_4$ and $\text{Ag}_2\text{VP}_2\text{O}_8$. Notably, the third material is a diphosphate material that as a class are much less frequently reported. Discharge behavior as well as mechanistic insights on the reduction of these materials will be presented.

Monday, September 9, 2013 08:00 PM[Sci-Mix \(08:00 PM - 10:00 PM\)](#)**Location: Indiana Convention Center****Room: Halls F&G****Tuesday, September 10, 2013 01:45 PM**[Advances in Batteries, Capacitors, and other Energy Storage Devices \(01:00 PM - 04:55 PM\)](#)**Location: Indiana Convention Center****Room: 123**

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Tuesday, September 10, 2013

296 - Toward fully plastic batteries: Electroactive polymer-carbon composite electrode as cathode material for rechargeable batteries

Burak Esat¹, besat@fatih.edu.tr, Muhammed Aydin². (1) Chemistry, Fatih University, Buyukcekmece/Istanbul, Turkey, (2) Chemistry, Gebze Institute of Technology, Gebze/ Kocaeli, Turkey

Fast recharging, flexible, small, light-weight, and environmentally compatible batteries with high power and energy capacities are required more than ever to meet the demands of today's booming portable device and electric vehicle industries. NiMH and Li-Ion batteries of today cannot provide these features simultaneously. Fully plastic batteries incorporating polymer electrodes and polymer electrolytes only in their cells are good candidates once suitable polymer electrodes and electrolytes are developed. To answer these challenges new redox- active polymer based electrodes with electro-active groups have been synthesized and characterized. Batteries with energy capacities 200 -300 mWh/g have been obtained. Recent advances in the field which utilize organic and polymeric electro - active materials are promising a bright future for polymer based rechargeable batteries.

[figure 1]

Monday, September 9, 2013 08:00 PM

[Sci-Mix \(08:00 PM - 10:00 PM\)](#)

Location: Indiana Convention Center

Room: Halls F&G

Tuesday, September 10, 2013 02:15 PM

[Advances in Batteries, Capacitors, and other Energy Storage Devices \(01:00 PM - 04:55 PM\)](#)

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Tuesday, September 10, 2013

297 - Thermal-induced decomposition roadmap of charged cathode material $\text{Li}_{1.2-x}\text{Ni}_{0.15}\text{Co}_{0.1}\text{Mn}_{0.55}\text{O}_2$ studied by synchrotron X-ray techniques

Chi-Kai Lin¹, cklin@anl.gov, Yang Ren², Ira Bloom¹, Zonghai Chen¹. (1) Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL 60439-4837, United States, (2) X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439-4837, United States

Lithium- and manganese-rich transition-metal layered-oxides (LMR-NMC), with composite structure $x\text{Li}_2\text{MnO}_3 \cdot (1-x)\text{LiMO}_2$, have been developed for future Li-ion battery (LIB) applications owing to their lower cost and high capacity. However, the safety should be carefully evaluated as the physical and electrochemical boundaries of LIBs have been aggressively pushed to achieve the high energy density (1,2). The safety characteristics are related to the exothermic reactions which can occur in charged batteries at elevated temperatures. Therefore, it is important to understand the thermally-induced, reaction pathways of the charged cathode material. Below, we discuss our recent study on the structural stability of the charged $\text{Li}_{1.2-x}\text{Ni}_{0.15}\text{Co}_{0.1}\text{Mn}_{0.55}\text{O}_2$ cathode.

Figure 1 shows the XRD patterns of charged $\text{Li}_{1.2-x}\text{Ni}_{0.15}\text{Co}_{0.1}\text{Mn}_{0.55}\text{O}_2$ in the enclosed cell with the presence of an electrolyte (1.0 M LiPF_6 in EC:EMC=3:7 by weight) as a function of temperature. Compared to the sample without electrolyte, dramatic electrolyte-induced structural changes are observed. This temperature of hexagonal structure ($R\bar{3}m$) conversion to a disordered LiM_2O_4 -type ($M=\text{Ni, Co, and Mn-rich}$) spinel ($Fd\bar{3}m$) is decreased from 266 to 234°C in the presence of electrolyte. Similarly, the temperature of disordered LiM_2O_4 -type spinel conversion to a M_3O_4 -type spinel is reduced from 298 to 234°C in the presence of electrolyte. Furthermore, M_3O_4 -type spinel reacts with electrolyte and decomposes to MO-type rock salt phase ($Fm\bar{3}m$) at 304°C. In addition, MO and M_3O_4 -type spinel continually decompose to MCO_3 till 400°C. When compared to the sample with solvent only, a retarded decomposition is observed. The formation temperatures of the MO and MCO_3 phases are reduced to 272 and 233°C, respectively, in the absence of salt. Considering that a new phase, MF_2 , initially appears at 210°C and its amount doesn't increase until above 320 °C, it may reveal that the salt-related decomposition products, such as MF_2 , retards the decomposition of M_3O_4 -type spinel and MO.

Monday, September 9, 2013 08:00 PM[Sci-Mix \(08:00 PM - 10:00 PM\)](#)**Location: Indiana Convention Center****Room: Halls F&G****Tuesday, September 10, 2013 02:35 PM**[Advances in Batteries, Capacitors, and other Energy Storage Devices \(01:00 PM - 04:55 PM\)](#)**Location: Indiana Convention Center****Room: 123**

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Tuesday, September 10, 2013

298 - High-voltage cathodes for lithium-ion batteries

Arumugam Manthiram, rmanth@mail.utexas.edu, Katharine Chemelewski. *Materials Science and Engineering, University of Texas at Austin, Austin, TX 78712, United States*

Lithium-ion batteries have enabled the revolution in portable electronics, but their adoption for transportation and stationary electrical energy storage requires the development of alternate materials with high energy and power with long cycle life at an affordable cost. The high-voltage spinel is an appealing cathode candidate in this regard, but its commercialization is hampered by capacity fade at elevated temperatures and variations and inconsistencies in performance depending on how it is made. Accordingly, this presentation will focus on a systematic examination of the various factors that influence the electrochemical performances of the high-voltage spinel cathodes. Specifically, the role of cation ordering, cation doping, surface planes/morphology, and surface composition on the electrochemical performances will be presented. Also, novel synthesis approaches to obtain specific morphologies and decouple the influence of the various factors will be presented.

Tuesday, September 10, 2013 03:05 PM

[Advances in Batteries, Capacitors, and other Energy Storage Devices \(01:00 PM - 04:55 PM\)](#)

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Ranjit Koodali, Yun Hu

Tuesday, September 10, 2013

299 - Probing electrochemical cycling stability of oxide cathode materials for Li-ion batteries by advanced electron microscopy

Miaofang Chi¹, chim@ornl.gov, Danna Qian², Christopher Fell², Shirley Meng². (1) Materials Science & Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, United States, (2) Department of NanoEngineering,, University of California San Diego, San Diego, CA 92093, United States

The transition metal (TM) intercalation oxides have been a major research interest as cathode materials for Li-ion batteries. During electrochemical charge and discharge cycling, these TM-oxides experience significant ion migration and elemental reduction/oxidation that produce large compositional variations and lattice distortions. Local structural properties (e.g., atomic occupancies, bonding, morphology, elemental and phase distributions at surfaces, interfaces, and bulk) are often the major parameters that determine the electrochemical behavior (e.g., capacity, rate capability, cycle life, etc.) in these materials. Advanced analytical electron microscopy (AEM), combining Z-contrast imaging, annular bright-field ABF) imaging, and electron energy-loss spectroscopy (EELS), offers ideal techniques for probing the local crystalline, chemical, and electronic structural evolution with atomic-scale resolution. In this presentation, recent studies of the local structural evolution in Li-excess layered oxides upon cycling will be reported. The results offer new insights into the structural changes, degradation pathways, and electrochemical processes of these materials, thereby providing guidance into possible routes for overcoming barriers that currently limit their electrochemical performance.

Tuesday, September 10, 2013 03:45 PM[Advances in Batteries, Capacitors, and other Energy Storage Devices \(01:00 PM - 04:55 PM\)](#)**Location: Indiana Convention Center****Room: 123**

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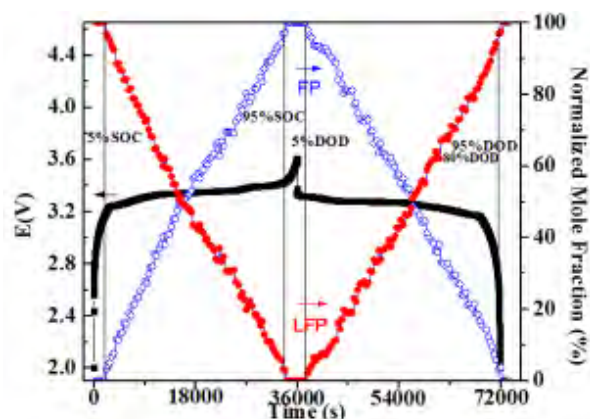
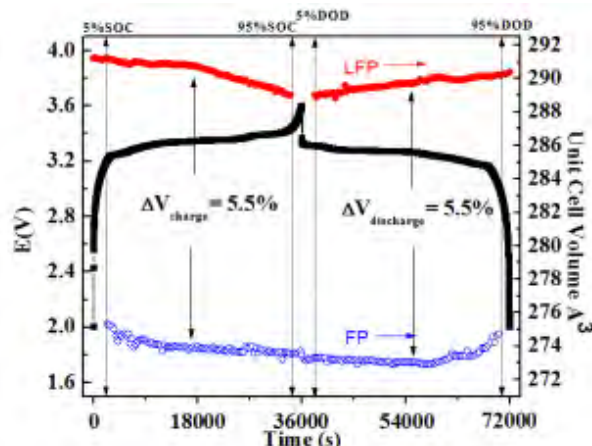
Ranjit Koodali, Yun Hu

Tuesday, September 10, 2013

300 - Study of phase changes about LiFePO₄ cathode in an 18650 commercial cell: An in situ time-resolved high energy synchrotron XRD study

Qi Liu¹, liuqi@iupui.edu, Yang Ren², Jian Xie¹. (1) Department of Mechanical Engineering, Indiana University Purdue University Indianapolis, indianapolis, IN 46224, United States, (2) X-ray Science Division, Advanced Photon Source, Argonne National Lab, Lemont, IL 60439, United States

Lithium iron phosphate is considered to be one of the most promising cathode materials of lithium ion battery. Though the performance of LiFePO₄ has been improved significantly, the mechanism of lithium ion insertion and extraction in FePO₄/LiFePO₄ is still not clearly understood. The understanding of the relationship between the structural changes and the electrochemical performance of LiFePO₄ is of paramount significance to the development of the LiFePO₄/C LIB cells. Here we investigated the in situ structure changes of electrodes in the commercial 18650 cells during the 1st charge/discharge process using the high energy synchrotron XRD. By utilizing the technique, the process of lithium intercalation in LiFePO₄ cathode during different conditions was revealed in detail, in situ and in a non-destructive manner. Our results show that the conventional LiFePO₄/FePO₄ two-phase reaction mechanism is not completely reached for the commercial cell. The single-phase transformation part of LiFePO₄ and FePO₄ exist, concurrent with two-phase reaction as theoretically predicted under nonequilibrium conditions.



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Wednesday, September 11, 2013

394 - Development of conductive binders for Si and tin anodes*Gao Liu, gliu@lbl.gov, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, United States*

Materials with high lithium storage capacity, such as silicon and tin based alloys, have recently been extensively studied for their potential applications as lithium-ion battery anodes. But the large-volume change associated with lithiation and delithiation severely hinders the practical employments. We report an effective solution to the volume-change by using conductive polymer binders. A class of new conductive polymers was developed through a combination of material synthesis, x-ray spectroscopy, density functional theory, and battery cell testing. Contrasting other polymer binders, the tailored electronic structure of the new polymer enables lithium doping under the operation condition of Si anode. The polymer thus maintains both electric conductivity and mechanical integrity during the battery operation. More importantly, this conductive polymer matrix is compatible with the lithium-ion slurry manufacturing process. This work implements the conceptual idea of combining binder and conductive additive into one material, solving the volume change problem of high capacity battery electrodes.

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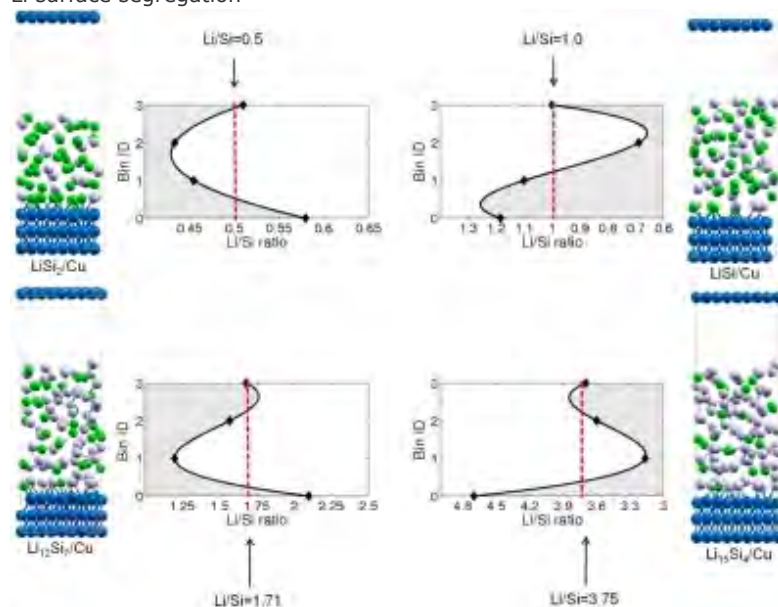
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395 - Understanding Li-ion batteries failure from first-principles calculations: The effect of lithiation on the Si/Cu interface in Si anodes

Maria E Stournara¹, maria_stournara@brown.edu, Priya Johari², **Yue Qi**³, yue.qi@gm.com, Vivek B Shenoy⁴. (1) Engineering, Brown University, providence, Rhode Island 02912, United States, (2) Engineering, Brown University, providence, Rhode Island 02912, United States, (3) General Motors, Warren, Michigan 30500, United States, (4) Engineering, Brown University, providence, Rhode Island 02912, United States

We study the effect of lithiation on the Si/Cu interface in Si anodes from first principles calculations. Through *ab initio* molecular dynamics (AIMD) and density functional theory (DFT), we calculate the ideal work of separation between the two slabs, the segregation of Li at the interfacial zone and predict the critical shear stress for sliding of the interface. We demonstrate that (a) increasing presence of Li at the interface is responsible for delamination of Si from the Cu substrate, (b) Li segregates at the interface by 22% for highly lithiated structures ($\text{Li}_{15}\text{Si}_4/\text{Cu}$) and that (c) lithium's presence at the interfacial zone results in sliding of the Li_xSi slab on Cu in agreement with experimental studies. To our knowledge, there has been no prior computational work that addresses the significant role of the interface from *ab initio* calculations. We believe that the results will provide a quantitative framework for the analysis of experimental measurements of deformation during lithiation/delithiation.

Li surface segregation



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Wednesday, September 11, 2013

396 - Electrochemical characterization Li-ion battery Sn anodes

Anne Co¹, co@chemistry.ohio-state.edu, Danny Liu¹, Jennifer Black², Amy Casaday¹. (1) Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH 43210, United States, (2) Oak Ridge National Lab, United States

Sn and its alloys exhibit promising energy storage capacity, with theoretical specific capacity of 959 mAh/g, and high electrical conductivity, for next generation lithium-ion batteries. In this paper, we describe the mechanism of Sn lithiation/delithiation on thin Sn films (30 to 200 nm) through an alloying/dealloying process, and the potential dependent SEI film formation examined using x-ray photoelectron spectroscopy and neutron depth profiling techniques.

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Wednesday, September 11, 2013

397 - Applications of carbide-derived carbon as electrodes for rechargeable lithium-ion batteries

Sun-Hwa Yeon, ys93@kier.re.kr, Kyu-Nam Jung, Sukeun Yoon, Kyoung-Hee Shin, Jae-Deok Jeon. *Energy Storage, Korea Institute of Energy Research, Deajeon 305-343, Republic of Korea*

Recently, there has been a considerable demand for the development of long-life lithium secondary batteries for energy storage systems. Carbonaceous materials have attracted great interest and are used as negative electrodes for lithium ion batteries due to more advantageous than lithium metal negative electrodes in terms of cycle performance by easy mobility of Li ion and safety. In order to increase energy density lithium alloys with Sn and Si are mainly studied as negative electrode, which exhibit three times of that of the graphite. However, these metal negative electrodes suffer significant mechanical disintegration due to the drastic volumetric changes during lithium insertion and extraction. Carbide-derived carbons (CDCs) possess tunable pore structures and narrow pore size distributions in the 0.5-2 nm range that can be formed through selective etching of crystalline metal carbides. This chemical etching method generates microporosity which affords high specific surface areas, large pore volumes, and large adsorption capacities. It also allows pore size matching to different molecules. Binary or ternary carbides such as TiC, SiC, ZrC, Mo₂C, and Ti₃SiC₂ are important precursors because the CDC porosities obtained can be tuned over a wide range with sub-Å accuracy by varying the chlorine etching temperature from 200-1200 °C. In this study, we introduce carbide-derived carbon(CDC) with tunable pore size and uniform pore structure, as positive and negative electrodes for secondary rechargeable lithium batteries.

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398 - Capturing the interface in Li-ion cells with heavy alkali dopants: Raman and X-ray techniques

Christopher J Patridge¹, christopher.patridge.ctr@nrl.navy.mil, Corey T Love², David E Ramaker². (1) Chemistry Division, NRC/Naval Research Laboratory, Washington, DC 20375, United States, (2) Chemistry Division, Naval Research Laboratory, Washington, DC 20375, United States

Li-ion electrochemical cells have shown marked improvements in capacity retention as well as safety using additives to polycarbonate electrolyte solutions. In a similar approach aimed at fundamental understanding, we have doped electrolyte solutions with heavy alkali cations (Rb^+ and Cs^+) with the goal of incorporating these cations into the surface films formed on both the cathode and anode active material known as the solid electrolyte interphase (SEI). These cations were chosen for their similar chemical reactivity as Li^+ and surface selectivity due to their much larger ionic radii than Li^+ . Chemical and local structure information is tracked using micro-probe Raman, X-ray photoelectron, and X-ray absorption spectroscopy as a function of electrochemical cycling. Findings suggest this approach could be a promising method to track the formation, growth, and chemistry of the SEI.

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Wednesday, September 11, 2013

399 - Mn dissolution induced surface related battery degradation and method to mitigate by simple surface treatment

Steve Harris¹, sjharris@lbl.gov, **Chen Li**². (1) Materials Science Division, Lawrence Berkeley National Lab, Berkeley, California 94720, United States, (2) Zee Aero, Mountain View, California 94720, United States

One of the critical challenges for lithium manganese oxide spinel-based batteries is the severe capacity fade due to Mn dissolution from the spinel, especially at high temperature.

In this talk, we will start from a model system with an inert Cu electrode and fluorine-free electrolyte, which eliminates the complexity of Li insertion in the active materials as well as the presence of HF. The goal is to elucidate the fundamental steps of how the presence of Mn in the electrolyte impacts the formation of SEI. How Mn dissolution influences the electrode surfaces and how the changes in surface chemistry harm battery long term viability will be discussed. Mn was found throughout the SEI, but not uniformly distributed. Also, the presence of Mn substantially increased the SEI formation and changed its composition and impedance. We take advantage of the fact that degradation films on both electrodes can be dissolved, and we remove the SEI contaminated with Mn by soaking the degraded electrodes in solvents. The relationships between these film properties and their effects on battery performance are described. We show a significant reduction in impedance from dissolving away these films.

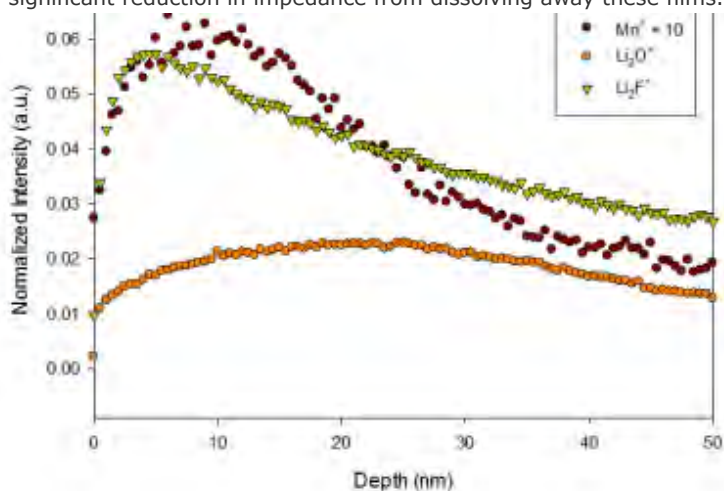


Figure1. TOF SIMS depth profiles showing Mn deposited on the graphite anode of a graphite/LMO full cell. Li₂O⁺ and Li₂F⁺ represent components from the SEI. The Mn⁺ intensities were multiplied by 10 to show the distribution trend.

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Wednesday, September 11, 2013

400 - High voltage electrolyte based on fluorinated compounds for 5V Li-ion chemistry

Zhengcheng Zhang, zzhang@anl.gov, Libo Hu, Huiming Wu, Khalil Amine. *Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL 60439, United States*

A new electrolyte based on fluorinated solvents was studied in a high voltage Li-ion cell using graphite as the anode and 5 V spinel $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ as the cathode. The electrolyte shows significantly enhanced voltage stability compared with the conventional electrolytes at elevated temperature (55 °C). Post-test study of the harvested cathode using FT-IR and SEM indicated that the buildup of organic decomposition product on the cathode surface previously observed with the conventional electrolyte is negligible for the fluorinated electrolyte. Additionally, the non-flammability of this fluorinated electrolyte will render improved safety of the Li-ion battery under abusive conditions.

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401 - Effect of electrolyte additives on solid electrolyte interphase properties in Li-ion batteries as analyzed by in-situ atomic force microscopy

Arthur V. Cresce, David R. Baker, **Selena M. Russell**, selena.russell.ctr@mail.mil, Kang Xu. Electrochemistry Branch, Power and Energy Division, Sensor and Electron Devices Directorate, U.S. Army Research Laboratory, Adelphi, MD 20783, United States

As lithium-ion batteries evolve toward higher cell voltage and capacity, developing detailed knowledge of the electrolyte/electrode interface is critically important. The solid electrolyte interphase (SEI) region plays a significant role in the reversibility and kinetics of the cell chemistry, e.g. by serving as the location for Li-ion solvation/desolvation and preventing persistent decomposition of the electrolyte while maintaining acceptable Li-ion transport. Additives to ethylene carbonate (EC) based electrolytes improve Li-ion battery performance, possibly by altering the physical or chemical properties of the SEI. While there is general agreement on the formation of the SEI on graphitic anodes from decomposed electrolyte, the morphology and composition dependence on additives is not well described. The inherent nature of the SEI, including its location on the electrodes, has impeded developing a well-supported understanding of its physical properties, composition, and true thickness.

Primarily using in-situ electrochemical atomic force microscopy (EC-AFM), we have systematically studied the relationship between the electrolyte and the resulting SEI formed on graphitic anodes. A key observation was that electrolytes with performance-enhancing additives formed thinner SEIs than additive-free electrolytes. Our results, coupled with the known benefits of these additives on battery performance, indicate that a more compact SEI is advantageous. SEI engineering through manipulation of additive chemistry could be the key to making high performance electrode-electrolyte pairs for high voltage Li-ion cells and perhaps alternative systems.

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402 - Electrolytes for lithium batteries from oligo(ethylene glycol) functionalized cyclophosphazenes and phosphazene oligomers

Kinkini Roy¹, kinkiniroy@polysci.umass.edu, Zhengcheng Zhang², Khalil Amine², E Bryan Coughlin¹. (1) Polymer Science & Engineering Department, University of Massachusetts, Amherst, Amherst, MA 01002, United States, (2) Chemical Science and Engineering Division, Argonne National Laboratory, Argonne, IL 60439, United States

There is a great interest in developing organic-inorganic oligomeric materials for use as electrolyte in lithium ion batteries. Polyphosphazenes are inorganic macromolecules that contain a backbone composed of alternating phosphorus and nitrogen atoms, and organic side groups can be attached to the backbone phosphorus atoms. They have extremely low glass transition temperature, are nonvolatile, nonflammable, and highly resistant to oxidation as well as efficient radical scavengers and flame quenching materials. Phosphazenes, with oligoethylene oxide side chains attached to the backbone of phosphorus atom, have numerous potential advantages as electrolytes. The synthesis and characterization of four different functionalized cyclotriphosphazenes are reported. Two different approaches were followed to synthesize mixed cyclotriphosphazenes. A mixture of all different varieties of mix-cyclotriphosphazenes was formed during the simultaneous addition of mixed alkoxides. Mainly two different mix-cyclotriphosphazenes were formed during the sequential addition. Small functionalized linear oligophosphazenes were also synthesized. All of these viscous liquids showed low glass transition temperatures. This suggests they are likely to be good candidates for electrolyte in lithium ion battery. Preliminary results showed these functionalized phosphazenes doped with 1.0M LiPF₆ has an ionic conductivity in the range of 10⁻⁴ S cm⁻¹ even at room temperature. We are expecting mixed phosphazenes will show higher conductivity.

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Wednesday, September 11, 2013

447 - Balanced approach for energy storage

Jun Liu, jun.liu@pnnl.gov, Pacific Northwest National Laboratory, Richland, WA 99352, United States

Energy storage covers many applications including portable electronics, transportation and grid scale storage. In general high energy density, high power density, long service life and good safety are desired, but there is no single technology that can be applied to all different applications. This talk will provide a comparison of the requirements and technologies for both transportation and stationary applications. Key aspects and progresses in Li-ion, Na-ion, Mg-ion chemistry, redox flow and Li-S batteries will be discussed. The importance and limitations of nanostructured materials and the challenges in understanding and controlling interfacial reactions on both cathode and anode sides will be addressed.

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448 - Anomalous manganese activation of a pyrophosphate cathode in sodium ion batteries: A combined experimental and theoretical study

Chansun Park¹, chanseonpark@kaist.ac.kr, Heejin Kim¹, Rara A. Shakoor², Eunjeong Yang¹, SooYeon Lim¹, Ramazan Kahraman², Yousung Jung¹, Jangwook Choi¹. (1) Department of EEWS, KAIST, Daejeon, Republic of Korea, (2) Department of Chemical Engineering, Qatar University, Doha, Qatar

Recently, sodium ion batteries (SIBs) have many attention paid to advantages such as the low price and abundance of sodium raw materials that are appropriable for large-scale energy storage applications. Herein, we report an Mn-based pyrophosphate, $\text{Na}_2\text{MnP}_2\text{O}_7$, as a new SIB cathode material. Unlike most Mn-based cathode materials, which suffer severely from sluggish kinetics, $\text{Na}_2\text{MnP}_2\text{O}_7$ exhibits excellent electrochemical activity at 3.8 V vs Na/Na⁺ with a reversible capacity of 90 mAh g⁻¹ at room temperature. It also shows a good cycle life and rate performance: 96% capacity retention after 30 cycles and 70% capacity retention at a c-rate (from 0.05C to 1C). These electrochemical activities of the Mn-containing cathode material even at room temperature with relatively large particle sizes are notable considering an almost complete inactivity of the Li counterpart, $\text{Li}_2\text{MnP}_2\text{O}_7$. Using first-principles calculations, we find that the significantly enhanced kinetics of $\text{Na}_2\text{MnP}_2\text{O}_7$ is principally due to the locally flexible accommodation of Jahn–Teller distortions aided by the corner-sharing crystal structure in triclinic $\text{Na}_2\text{MnP}_2\text{O}_7$. By contrast, in monoclinic $\text{Li}_2\text{MnP}_2\text{O}_7$, the edge-sharing geometry causes multiple bonds to be broken and formed during charging reaction with a large degree of atomic rearrangements. We expect that the similar computational strategy to analyze the atomic rearrangements can be used to predict the kinetics behavior when analyzing new cathode candidates.

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449 - Development of high energy density Li-organic redox flow battery

Wei Wang, wei.wang@pnnl.gov, Wu Xu, Xiaoliang Wei, Lelia Cosimbescu, Daiwon Choi, Vincent Sprenkle. Pacific Northwest National Laboratory, Richland, WA 99354, United States

Here we report the development of nonaqueous high energy density Li-organic redox flow battery (LORFB) based on a modified redox active organic molecule as the positive electrolyte and lithium metal as the negative electrode. Molecular modification of quinone-based and ferrocene-based organic materials have demonstrated significantly improved solubility in common organic solvent, enabling the organic molecules to function as energy bearing active materials in the positive electrolyte. The synthesis and the electrochemical study of the two organic materials and the performance of the nonaqueous flow cell using the modified organic redox couple as positive electrolyte will be reported.

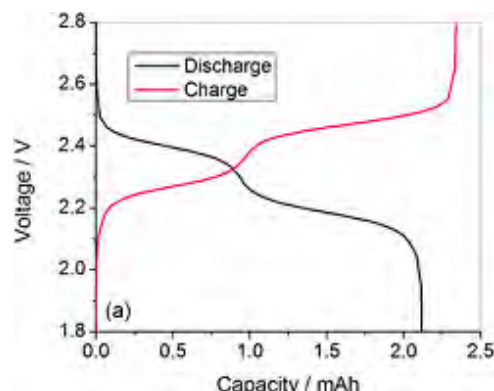


Figure 1. Cell voltage profile of a LORFB with 0.25 M modified Anthriquinone in 1.0 M LiPF₆/PC solution as positive electrolyte and lithium foil as negative electrode.

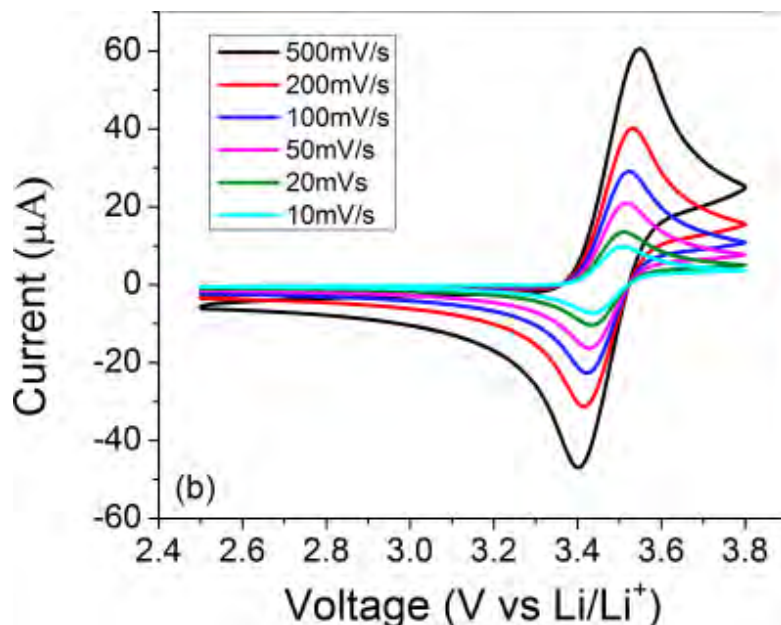


Figure 2. CV of a modified Ferrocene-based organic couple.

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450 - Electrodeposition of metal-air battery cathodes: Fabrication, characterization, and electrochemistry

Amy C Marschilok^{1,2}, amy.marschilok@stonybrook.edu, Shu Han Lee³, Esther S Takeuchi^{1,2,4}, Kenneth J Takeuchi². (1) Department of Materials Science and Engineering, Stony Brook University, Stony Brook, NY 11794, United States, (2) Department of Chemistry, Stony Brook University, Stony Brook, NY 11794, United States, (3) Department of Chemical and Biological Engineering, University at Buffalo, Buffalo, NY 14260, United States, (4) Global and Regional Solutions Directorate, Brookhaven National Laboratory, Upton, NY 11793, United States

Metal air batteries offer the opportunity for significant energy density improvements relative to current battery technologies. Air cathodes typically require a catalyst, conductive additives, binder, and current collector to function effectively. Each component plays a critical role, where the current collector provides support and conductivity, the binder provides physical adhesion, and the catalyst facilitates the oxygen reduction process at the cathode. Access of the catalyst particle to oxygen is critical, so the cathode porosity must be appropriately tuned. Typically, electrodes are fabricated using physical mixing methods, where limitations include poor interparticle contact and poor access of the interior catalyst particles to oxygen.

Fabrication of a composite air cathode via electrodeposition will be discussed. The first layer consists of a current collector substrate, which can be two dimensional (planar) or three dimensional in design. The second layer consists of a conductive polymer, which is conformally coated onto the current collector substrate via electrodeposition. The third layer consists of catalyst particles, dispersed on the polymer layer via a second electrodeposition process.

The deposition processes will be studied using both electrochemically and non-electrochemically based methods. A quartz crystal microbalance will be used to quantify the deposits. In addition, catalyst content will be quantified using inductively coupled plasma-optical emission spectroscopy. Microscopy will also be used to evaluate morphology of the composite electrodes. Impedance spectroscopy and voltammetry will be employed to evaluate electrochemical properties of the composite electrodes, including oxygen reduction activity.

Advantages of the electrodeposition fabrication method will also be described. Three-dimensionally structured composites can be easily generated via use of three dimensional substrates. All of the catalyst nanoparticles are positioned on the outer surface of the composite electrode, allowing facile access of oxygen gas molecules to the catalyst particle surfaces. Finally, the conductive polymer provides added conductivity and improved stability to the composite.

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451 - Li intercalation capacity of Fe-phthalocyanine

Ramos-Sanchez Guadalupe, gramos@neo.tamu.edu, Perla B Balbuena. Chemical Engineering Department, Texas A&M University, College Station, Texas 77843, United States

Formation of intercalation compounds providing enhanced energy density and excellent rechargeability is promising for secondary Li batteries. In this work we used DFT to determine the intercalation capacity of β -FePc. This system has shown significant capacity of intercalation up to 43 Li atoms, and excellent stability to charge/discharge cycles. This behavior is connected to the chemical processes occurring during the intercalation; however molecular detail has not been reported so far. Two functionals were used, RPBE and PBE-D2 where the D2 stands for the inclusion of a semiempirical treatment of vdW interactions. Using PBE-D2 functional an almost constant potential of 2 V during discharge was observed, in the other hand using standard DFT the intercalation voltage rapidly decreases as consequence of the tendency of Lithium atoms to attach to either the upper or lower FePc molecules, while using PBE-D2 functional the Li atoms remain in the middle of them. The Li atoms intercalated lost partial electronic density and became positively charged (+0.83 average charge) which indicates a charge transfer intercalation mechanism. The charge donated by the Li atoms is accepted by all the FePc constituents atoms, however is the Fe which suffers the most drastically charge change. In the free FePc the Fe atom charge is +1.2, from 1 to 6 Li atoms the charge changes gradually to +0.2, remaining in this value up to 14 atoms, and finally reaching negative values with 21 Li atoms intercalated. Other atoms receive electronic charge from Li; however the central Fe has the capacity to donate or withdraw atoms in order to keep the structural integrity of the system. Up to 29 intercalated Li atoms no bond rupture in the FePc or dramatic change in the unit cell size or shape was observed.

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452 - Low cost, abundant, defective materials for large scale electrical energy storage

Dan Steingart, steingart@princeton.edu, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ 08544, United States

Electrochemical energy storage induces headaches in industrialists for the same reason it provides such fertile ground for academics: a working, rechargeable battery represents a tight coupling of multiphase phenomena across mechanical, thermal and electrical domains. The properties of battery materials have been well classified in the literature in an anatomical fashion, but systematic treatments of the composite battery electrode and complete storage device have been less rigorous. By treating every cycle of the battery in the materials science framework of process-performance-properties, we are exploiting the very problems that limit low cost materials to primary batteries. By linking sub micron phenomena to systematic consequences through in situ measurements, we are able to demonstrate packaging and cycling methodologies which may lead to low cost, high cycle life grid scale batteries based on Zinc and MnO₂.

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453 - Fundamentals and structure designs for Na-ion battery anodes

Liangbing Hu, binghu@umd.edu, Materials Science and Engineering, University of Maryland CollegePark, College Park, MD 20782, United States

Na-ion batteries are attracting much interest due to their potential low-cost applications. I will present our recent results on tin (Sn) anodes with rational designs. Improved cycling performance will be presented. In-situ TEM studies show the importance of surface coating on the improved performance. I will also present some results related to mechanical properties of SEI in Na-ion anode based on ex-situ and in-situ AFM.

Wednesday, September 11, 2013 03:45 PM[Advances in Batteries, Capacitors, and other Energy Storage Devices \(01:00 PM - 05:15 PM\)](#)**Location: Indiana Convention Center****Room: 123**

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Wednesday, September 11, 2013

454 - Enhanced lithium ion battery via biological engineering**Scott J Riley**, Sriley6@umbc.edu, Chemistry, UMBC, Catonsville, Maryland 21228, United States

In today's modern world the demand for more efficient forms of energy storage is increasing everyday. Electrochemical cells are the most widely used form of portable energy storage and is growing to become the most highly used large scale energy storage. From mobile devices to cars, batteries are integrated into many facets of daily life, but are reaching their limit. While batteries have been improving over the years the growth is slow and staggered. An improvement similar to the discovery of lithium ion batteries needs to be made in order to keep up with demand. This improvement can be made by interfacing biology and batteries.

My research focuses on using a bio-inspired approach to address battery performance. We use the technique of phage display to isolate solid binding peptides (SBP) that bind specifically to Lithium Nickel Cobalt Oxide (LNC). Once SBPs are isolated for LNC they will be heterologously expressed in *E. coli*

and combined with carbon nanotube binding peptides. These multifunctional peptides will be used to bio-tether conducting CNTs with electro active materials and thus make better conducting hybrid electrodes. This new model for the electrode would enhance multiple aspects of battery performance including capacity, cyclability, and power.

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Thursday, September 12, 2013

505 - Pseudocapacitive energy storage in 2D Nb₂O₅-graphene nanocomposites

Guillaume Muller, Hyungseok Kim, Xavier Petrissans, Veronica Augustyn, **Bruce Dunn**, bdunn@ucla.edu. Department of Materials Science and Engineering, University of California, Los Angeles, Los Angeles, CA 90095-1595, United States

Capacitive energy storage is distinguished from other types of electrochemical energy storage by short charging times, the ability to deliver significantly more power than batteries and long cycle life. A key limitation to this technology is its low energy density and for this reason there is considerable interest in exploring pseudocapacitive charge storage mechanisms in which fast and reversible redox reactions lead to energy densities which are at least an order of magnitude larger than traditional double layer capacitors. The research reported here builds on our recent work in which Nb₂O₅ exhibited the electrochemical features of a pseudocapacitive material despite having charge storage result from lithium ion insertion in the bulk. In this study, we prepared nanocomposites comprised of Nb₂O₅ platelets and graphene sheets. By using platelets of the pseudocapacitor material, we retain the 2D morphology of each component and this seems to be beneficial for the electrochemical properties. The material possesses high capacitance and excellent rate capability. The addition of RGO enhances charge transfer reactions with Nb₂O₅ and the composite is able to maintain high capacity at high sweep rates. The development of such 2D systems represents an interesting direction for creating electrochemical capacitor materials with improved levels of energy density.

Thursday, September 12, 2013 08:00 AM[Advances in Batteries, Capacitors, and other Energy Storage Devices \(08:00 AM - 11:25 AM\)](#)**Location: Indiana Convention Center****Room: 123**

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Thursday, September 12, 2013

506 - High performance heterogeneous catalysis at ultrashort contact time for fuel cell cathode air using microfibrinous entrapped catalysts

Qiang Gu, QZG0001@AUBURN.EDU, Bruce Tatarchuk. Chemical Engineering, Auburn University, Auburn University, AL 36849, United States

Microfibrinous Entrapped Catalyst (MFEC) manufactured from 8 μm diameter nickel fibers were engineered into pleated heterogeneous reactor to improve catalytic performance compared with conventional packed bed and monolith reactors. MFEC entraps small particles (150-200 μm) by the sinter-lock structure of metal fibers, which significantly improves inter phase mass transfer rate. Conventional reactors usually operate with contact time less than 1s. MFEC reactors were able to reduce the contact time to micro seconds, while maintaining similar catalytic performance. This gives MFEC huge advantages in terms of weight and volume saving, since the conventional meter-long reactors were shortened to millimeter thick material sheets.

In this research, MFEC reactors were investigated under conditions of high temperature (100-200C) and high face velocities (10-30 m/s). These high face velocities results in interlayer contact times of 67-200 μsec . Precious metal (1% Pd, 1% Ag) and transition metal (%10 Mn) catalysts were impregnated on entrapped particles (e.g. $\gamma\text{-Al}_2\text{O}_3$) using incipient wetness method. Catalytic performance showed that a high level of ozone decomposition was achieved with a significant reduction of catalyst consumption compared with monolith. Detailed reaction kinetics were analyzed based on numerically determined flowed types in the reactor. Besides, several aspects including humidity, system pressure and aging have been investigated for affection on the catalytic performance.

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Thursday, September 12, 2013

507 - Natural cellulose fiber as substrate for supercapacitor with extra ion diffusion pathway

Zhe Gui¹, zgui@umd.edu, Hongli Zhu², Eleanor Gillette¹, Junkai Hu¹, Liangbing Hu², Sangbok Lee¹. (1) Department of Chemistry, University of Maryland College Park, college park, Maryland 20740, United States, (2) Department of Materials Science and Engineer, University of Maryland College Park, college park, Maryland 20740, United States

Cellulose fibers with porous structure and electrolyte absorption properties are considered to be good potential substrate for the deposition of energy material in energy storage devices. In this study, we directly proved this idea by comparing a series of hybrid electrodes based on home-made cellulose paper integrated with CNTs, and electrodeposited with MnO₂ for supercapacitor. Paper was prepared from pure natural cellulose fibers without any additive by filtration method. Conformal CNTs layers were fabricated through simple solution dip and dry method, and MnO₂ was prepared by electrochemical deposition. Atomic layer deposition (ALD) of Al₂O₃ was used to cover the fibers for the preparation of substrates with limited electrolyte absorption for comparison. Configurations designed with different numbers of ion diffusion paths were compared and results show that cellulose fibers as substrate also function well as interior electrolyte baths and effectively facilitate the ion diffusion process. To further optimize the electrode, another CNTs layer was deposited on the top of MnO₂ resulting in the configuration of Paper/CNTs/MnO₂/CNTs. Both extra ion diffusion and electron transfer pathways were activated in this hybrid structure, showing superior supercapacitive performance than other samples with limited charge transfer paths. This paper highlights the merits of the mesoporous cellulose fibers as substrates for supercapacitor electrode, in which the water-swelling effect of the cellulose fibers can absorb electrolyte, and the mesoporous internal structure of the fibers can provide extra pathways for ions to diffuse to the energy materials.

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Thursday, September 12, 2013

508 - Semiconductor nanowire-arrayed electrodes for supercapacitors

Yat Li, yatli@ucsc.edu, Department of Chemistry and Biochemistry, University of California Santa Cruz, Santa Cruz, California 95064, United States

This talk will present highlights of the latest results of studies directed at developing semiconductor nanowires (e.g., TiO₂, TiN, and VO), as well as nanowire heterostructures (e.g., TiO₂/MnO₂ and TiO₂/C core-shell nanowires) as electrode materials, which show significantly enhanced performance and stability in applications for supercapacitors. The enhanced performance and cycling stability of the nanowires are attributed to improved electrical conductivities. These one-dimensional nanowires and core-shell nanowires were grown directly on flexible conductive substrates, which not only provide good strain accommodation, but also enable the fabrication of flexible solid-state supercapacitor devices without the need of a binder.

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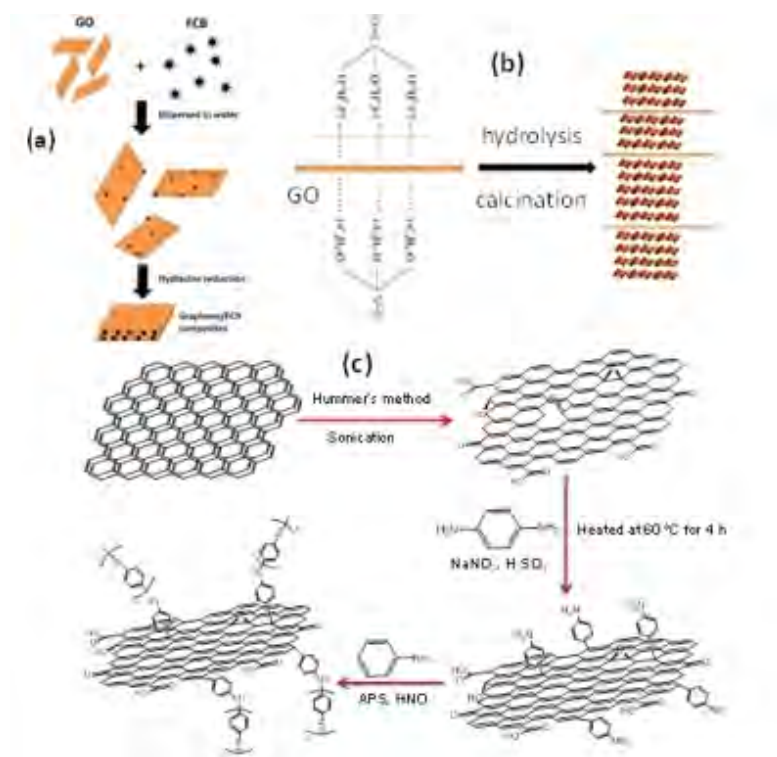
Thursday, September 12, 2013

509 - Graphene-based composites as electrochemical supercapacitors

Zhefei Li, zhefli@iupui.edu, Jian Xie. Department of Mechanical Engineering, Indiana University Purdue University Indianapolis, Indianapolis, Indiana 46202, United States

Owing to the increasing power requirements for electric vehicles, tremendous work has been devoted to supercapacitors with high power density, energy density, and rate performance. Electrochemical supercapacitors are attractive because of their better cycling performance and higher power density as compared to Lithium-ion batteries. Graphene, a 2-Dimensional structure of sp^2 carbon atoms, has attracted much attention recently. Due to its large surface area, excellent conductivity, and good stability, graphene can be incorporated in the composites materials to enhance the performance.

In the present work, graphene composites with functionalized carbon black, polyaniline, and V_2O_5 have been prepared via facile chemical routes. The schematic illustration of synthetic methods is shown in Figure 1. The resulting composites exhibited improved performance compared to graphene, functionalized carbon black, polyaniline, and V_2O_5 alone. For instance, the graphene/FCB composite electrode showed a specific capacitance of 168 F/g in aqueous electrolyte (1 M H_2SO_4) and 137 F/g in organic electrolyte (1.2 M $LiBF_4$) at 1 A/g, much higher than that of graphene (82 F/g and 65 F/g). Graphene/ V_2O_5 composites showed a specific capacitance of 427 F/g at 5 mV/s scan rate, while the capacitance of pure V_2O_5 is only 274 F/g. Covalently-grafted polyaniline/GO composites possessed a specific capacitance of 387 F/g at 1 A/g and longer cycle life than pure polyaniline. The excellent performance suggests a good synergistic effect between graphene and supporting materials.



Monday, September 9, 2013 08:00 PM

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Ranjit Koodali, Yun Hu

Thursday, September 12, 2013

511 - Mechanism of oxidized redox shuttle reduction at graphite or LTO anodes

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Redox shuttle compounds can help improve the safety of lithium ion batteries by preventing overcharge. During an overcharge event at a low enough C-rate, redox shuttle compounds limit the cathode potential as they are oxidized. They then diffuse to the anode, where they are reduced. A central question concerning the action of redox shuttle compounds concerns the mechanism of reduction of the oxidized redox shuttle compound, since the solid-electrolyte interphase (SEI) layer that is present on carbon anodes is supposed to be electrically insulating. At least two theories have been proposed for the reduction of the oxidized redox shuttle compound at the anode: electron tunneling through the compact inorganic SEI layer after transport through the organic SEI layer, perhaps aided by molecular imprinting, or reaction with lithium metal plated on the anode as its potential drops below 0 V vs. Li⁺/Li during overcharge. In this investigation, reference electrodes will be inserted into lithium ion batteries with lithium iron phosphate (LFP) cathodes and either graphite or lithium titanium oxide (LTO) anodes to measure the cathode and anode potentials during overcharge. This data should help clarify the mechanism of the reduction of the oxidized redox shuttle 1,4-di-tert-butyl-2,5-dimethoxybenzene at the anode.

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Thursday, September 12, 2013

512 - Synthesis of boron carbide, zirconium carbide, and niobium carbide nanofibers through electrospinning followed by carbothermal reduction

Jennifer S Atchison, jennifer.atchison@INM-gmbh.de, Volker Presser. *Energie Materialien, INM Leibniz Institut für Neue Materialien, Saarbrücken, Saarland 66123, Germany*

High surface area materials with tunable porosity have attracted significant interest. In particular, hierarchic porous materials are highly desirable that combine micro-, meso- and macro pores for applications based on the formation of an electrical double-layer. Such applications include electrodes in electrical double-layer capacitors (EDLC, commonly called supercapacitors) and capacitive de-ionization (CDI).

Composite electrospun nanofibers whose high aspect ratio, controllable processing, and wide selection of chemistries an attractive option for the rational design of high surface area electrodes used in EDL devices. As shown recently, carbide-derived carbons (CDC) can be electrospun and have been demonstrated to have tunable pore size distributions with specific surface areas up to 1800 m²/g. Sol-gel synthesis followed by carbothermal reduction is a well established route to carbide synthesis and electrospinning the solution with a carrier polymer while retarding the gelling process has been shown to produce fibers that are composed of carbide crystal domains bound together by amorphous carbon.

This work extends the synthesis procedure beyond the previous work which was exclusively limited to SiC and TiC. Specifically, the parameters and chemistry for electrospinning carbide-carbon composite nanofiber assemblies is established for synthesizing boron carbide, zirconium carbide, and niobium carbide electrospun nanofibers. The nanofiber morphology, fiber diameter distribution, specific surface area, and crystallinity have been studied. These metal carbide/carbon composite fiber mats are the foundation materials for porosity engineering as well as the support for the introduction of macro pore fillers designed to improve the volumetric energy density and the rate handling ability while maintaining the reliability and efficiency of EDL electrodes.

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